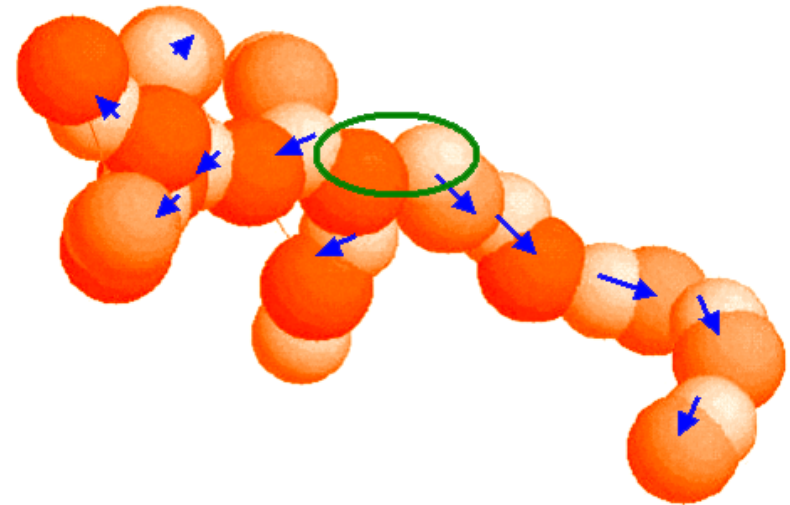


# Interstitialcy Theory of Liquids and Glasses

A. V. Granato, University of Illinois, NSF DMR-0138488

The recent discovery of inhomogeneous string-like collective motion in liquids and glasses has made possible a discrimination between different theories of condensed matter. By displaying only those atoms with displacements larger than a critical amount, the “strings” are emphasized in the figure. We have shown (K. Nordlund, Y. Askenazy, R.S. Averback and A.V. Granato – submitted to Phys. Rev. Lett.) that the strings are interstitial defects. These findings strongly support the Interstitialcy Theory of Condensed Matter (ITCM), and also provide a straightforward means of defining and identifying the interstitials in liquids and glasses. If an atom is in the string, it is a part of the interstitialcy configuration.



*Atomic displacements following interstitial introduction in quenched amorphous copper. Light (small) spheres represent pre-insertion positions; darker (larger) spheres represent final relaxed positions. All plotted atoms were displaced more than  $0.7\text{\AA}$  and those with a darker shade moved more than  $1.2\text{\AA}$ . The green ellipse highlights the location of the interstitial atom. The blue arrows indicate the direction of collective motion.*

University physics textbooks routinely describe three states of matter: solid, liquid, and gas. The treatment of solids and gases is exhaustive. Conspicuous by its absence is any substantive discussion of the liquid state, even to this day. This is true in spite of the fact that water covers 75% of the planet and that the liquid state is the basis of life itself.

Historically, the study of gases came first. Chemists and physicists of the late 1800's were able to establish quantitative and universal relationships between the temperature, volume, and pressure of matter in this state. With the advent of x-ray techniques and the birth of quantum mechanics in the early 1900's, scientists increased their knowledge of solids as well. Students now learn details about crystal structures and other properties of solids thanks to contributions from luminaries like Planck, Einstein, and Debye. Still, there is no systematic or rigorous treatment of liquids.

One notable finding for real crystals at temperatures above absolute zero (even for pure elements) is that not all atoms are on predicted lattice sites. "Defects" are produced by thermal fluctuations. One – the vacancy – occurs when an atom is missing from its assumed position. Another – the interstitial – exists when an extra atom appears in the lattice. It turns out that for crystalline materials the properties of the vacancy dominate. This is because the concentration of these defects is roughly 10-100 times higher than of interstitials just below the melting temperature.

However, according to the Interstitialcy Theory of Condensed Matter (ITCM), all this changes at the melting temperature. Here the situation is reversed, with the number of interstitial defects growing dramatically relative to the number of vacancies. Because interstitials weaken the crystal (loss of rigidity and lower viscosity) the material "melts." The ITCM can even explain the magnitude of energy required to melt a unit mass of any given element at its melting temperature – an observation noted in 1893, known as Richard's Rule – but heretofore unexplained.

# Interstitialcy Theory of Liquids and Glasses II

A. V. Granato, University of Illinois, NSF DMR 01-38488

## Education:

- Two Visiting Scientists
  - D.M. Joncich, Ph.D. (full time)
  - J.T. Holder, Ph.D. (part time)
- Three Visiting Physics Professors
  - D. M. Zhu, Ph.D. (part time)
  - B. Igarashi, Ph.D. (part time)
  - V. A. Khonik, Ph.D., D.S. (part time)
- One Graduate Student
  - A.S. Bains (Kinetics of mechanical relaxation near the glass temperature)
- Four undergraduates
  - A. Karmis (low-T thermal conductivity)
  - A. Pompe (high-T shear modulus)
  - A. Niemerg (high-T electrical resistivity)
  - T. Lim (computer support)

## Societal Impact:

Metallic glasses hold great potential for the future. These amorphous materials are hard, corrosion-resistant, ductile, and twice as strong as conventional alloys. In addition, they can be produced in molds – a process which dramatically reduces material waste and adverse environmental impact during fabrication.

Current applications include low-loss transformers, fiber optics, high-performance specialty coatings, solar cells, and materials for radioactive waste storage.

The Interstitialcy Theory of Condensed Matter provides the only fundamental microscopic model for the properties of these glasses.

**IMPACT:** We address this topic in two areas – basic science and practical applications.

**Basic Science** – From the standpoint of basic research the ITCM program is significant.

According to poll of scientists conducted by Physics World magazine, glassy materials ranked as one of the top ten unsolved problems in physics. (PhysicsWeb Survey, 11/99)

We also quote Nobel Laureate Philip W. Anderson – “The deepest and most interesting unsolved problem in solid state theory is probably the theory of the nature of glass and the glass transition. This could be the next breakthrough in the coming decade.” (1995)

In general, one can describe the properties of matter in two broad categories: equilibrium thermodynamic constants and kinetic effects. The former refers to properties measured in the “steady state,” under conditions of constant temperature, pressure, stress, etc. (These quantities may all be derived from an entity known as the Gibb’s Free Energy.) The latter describes responses of the system with time after externally imposed stimuli.

Typical thermodynamic constants include the density (mass/volume), thermal expansion (length change with temperature), compressibility (volume change with pressure), and specific heat (temperature change with energy). Some important kinetic effects are electrical resistivity (current flow with voltage), thermal conductivity (heat flow with temperature gradient), and diffusion (mass migration with temperature and/or stress).

To date, the ITCM has successfully predicted many equilibrium thermodynamic properties of metallic glass compounds. We are now in the process of predicting and measuring the kinetic properties of these unique materials as well.

Glassy materials have been the subject of intense investigation for the past fifty years. Unfortunately, the researchers in this field work in different domains of temperature, pressure, external stress, and measurement parameters. In many cases, they do not even use the same terminology to describe their findings. In addition, current methods to produce metallic glasses are empirical, typically involving trial and error to identify good “glass formers.” Results are explained in terms of “energy landscapes” or “free volume.”

The ITCM, on the other hand, provides a unified framework and vocabulary to describe all these results. It is also the only physical theory to describe the properties of amorphous materials quantitatively rooted in basic science.

## **Practical**

Defense applications abound – DARPA has invested \$30 million to accelerate the growth of this technology for armaments, submarines, and aircraft. Unfortunately, their research funding is often targeted for more immediate, applied results. There have also been many new, spin-off companies, eager to apply the unique properties of glass technology for profit. Continued NSF funding for the ITCM is critical to the success of all these efforts.